

Combined Influence of Off-diagonal System Tensors and Potential Valley Returning of the Optimal Path

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Abstract

The two-dimensional barrier passage is studied in the framework of Langevin statistical reactive dynamics. The optimal incident angle for a particle diffusing in the dissipative non-orthogonal environment with various strengths of coupling between the two degrees of freedom is systematically calculated. The optimal diffusion path of the particle in a non-Ohmic damping system is revealed to have a probability to return to the potential valley under the combined influence of the off-diagonal system tensors.

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I. INTRODUCTION

The problem of escaping from a metastable state potential is of ubiquitous interest in almost all scientific areas in particular the study of nuclear reactions. The related reactive system is usually modeled within the framework of one-dimensional (1D) standard Brownian motion [1–4]. However, since it leaves out the correlation between different degrees of freedom while many processes obviously involve more than one degree of freedom, the classical 1D model fails to describe satisfactorily the dynamical evolving of a real reactive process. Basing on these considerations we have recently generalized the 1D model to the two-dimensional (2D) case by analyzing a set of coupled generalized Langevin equation[5, 6].

It has been shown that the diffusion in a 2D potential energy surface (PES) includes nutritious useful information of the reactive dynamics such as there exists an optimal incident angle (or an optimal path) for the particle to obtain its maximum probability to surmount the PES barrier. This provides a convenient way to understand many stochastic dynamical processes such as the fusion of massive nuclei and even the synthesis of super-heavy elements because one can easily estimate the reactive probability of a particle by tracing its footprint along the optimal path.

Moreover, It is also revealed that the non-orthogonality of the PES and the off-diagonal system parameters is very important in determining whether a reactive processes can be easily accomplished or not. Although this was mentioned in some previous studies[7, 8], less effort has been made to give a thorough investigation. In particular, no research has based directly on the optimal incident angle as far as we have known. Therefore it is very meaningful to seek for more detailed information on this subject.

In this paper, motivated by the interest of better understanding the 2D reactive dynamics, we present a relatively systematic study of the optimal incident angle which enables the particle to surmount the barrier with maximum passing probability. Firstly, in Sec. II a large number of Langevin calculations are performed in the Ohmic damping case by simultaneously varying the off-diagonal term of the system tensors. Secondly, in Sec. III, influence of the non-orthogonality of the system tensors on the non-Ohmic damping diffusion process is discussed where a startling potential valley returning behavior of the optimal path is witnessed. Sec. IV is a summary of our conclusion in which also the implicit application of this work is discussed.

II. COMBINED INFLUENCE OF OFF-DIAGONAL SYSTEM TENSORS

In brief, we begin with the optimal incident angle defined in our previous study by tracing the minimum value of critical initial velocity v_0^c in a 2D Ohmic damping barrier surmounting process[5]. It reads

$$\phi_m = \arctan \left(\frac{m_{12}(\beta_{22}a + \omega_{22}) - m_{22}(\beta_{12}a + \omega_{12})}{m_{11}F_1(a) + m_{12}F_2(a)} \right) \quad (1)$$

where $F_j(a)$ s, ($j = 1, 2$) are the related functions derived in the process of Laplace solving the coupled Langevin eqnarray $m_{ij}\ddot{x}_j(t) + \beta_{ij}\dot{x}_j(t) + \omega_{ij}x_j(t) = \xi_i(t)$. Expressions of them are

$$\begin{aligned} F_1(a) &= m_{22}a^2 + \beta_{22}a + \omega_{22}, \\ F_2(a) &= -m_{12}a^2 - \beta_{12}a - \omega_{12}, \end{aligned} \quad (2)$$

with a the largest analytical root of

$$\begin{aligned} &(\det m)s^4 + (m_{11}\beta_{22} + m_{22}\beta_{11} - 2m_{12}\beta_{12})s^3 \\ &+ (\det \beta + m_{11}\omega_{22} + m_{22}\omega_{11} - 2m_{12}\omega_{12})s^2 \\ &+ (\beta_{11}\omega_{22} + \beta_{22}\omega_{11} - 2\beta_{12}\omega_{12})s + \det \omega = 0 \end{aligned} \quad (3)$$

the symbols with subscripts such as m_{12} are the components of inertia (m_{ij}), friction (β_{ij}) and potential-curvature (ω_{ij}) tensors respectively, “det” denotes the determinant of each tensor. In the Ohmic damping case, all the system tensors in the Langevin eqnarray can be considered as invariable constants and correlations of the two components of the random force $\xi_i(t)$ obey the fluctuation-dissipation theorem $\langle \xi_i(t)\xi_j(t') \rangle = k_B T m_{ik}^{-1} \beta_{kj} \delta(t-t')$, where k_B is the Boltzmann constant and T the temperature.

Noticing, Eq. (1) implicitly contains the off-diagonal term of the system tensors. This implies the non-orthogonality of the system tensors is an important factor in determining the reactive probability of a particle. A combined control of them on the optimal incident angle can be expected. The primary purpose of this work is then to obtain some comprehension on this phenomenon.

In the calculations here and following, we rescale all the variables so that the dimensionless unit is used. In Fig. 1, the optimal incident angle is plotted as a function of various off-diagonal parameters ($\mathbf{p}_{\text{off-dia}}$). From which we can see that the optimal incident angle varies

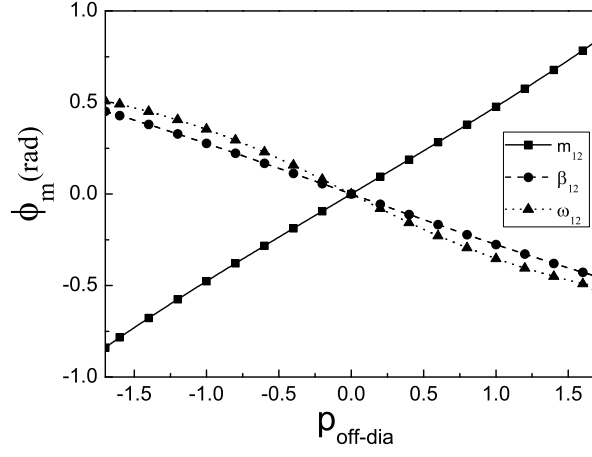


FIG. 1: Optimal incident angle as a function of various off-diagonal parameters ($p_{\text{off-dia}}$). When one is varying the other two remains zero. Other parameters used here are: $m_{11} = 1.5$, $m_{22} = 2.0$, $\beta_{11} = 1.8$, $\beta_{22} = 1.2$, $\omega_{11} = -2.0$, $\omega_{22} = 1.5$.

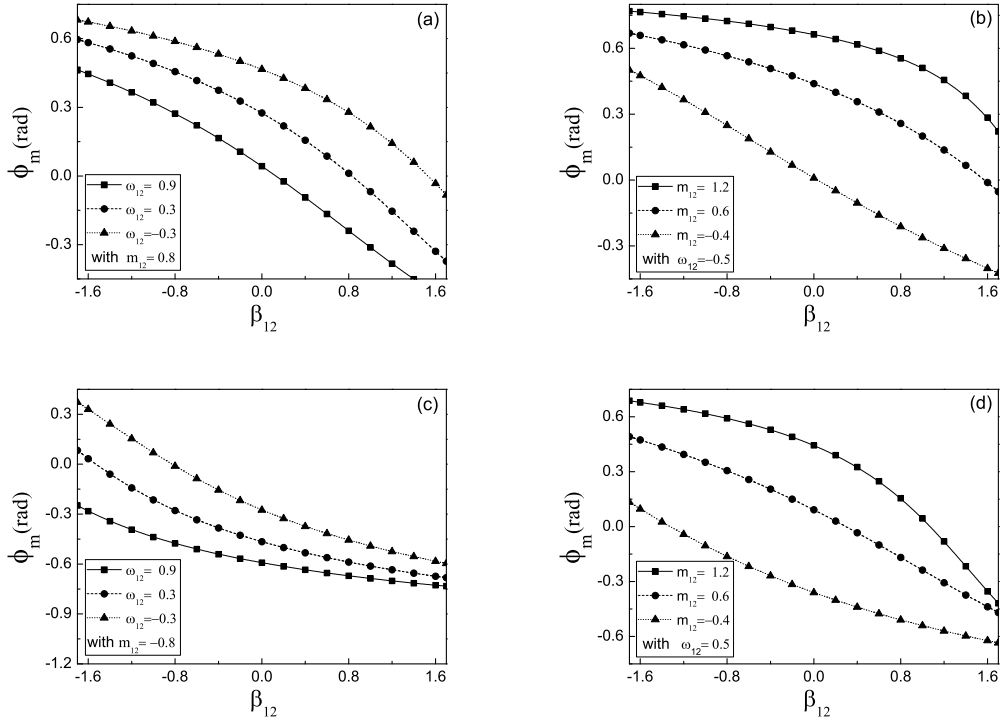


FIG. 2: Optimal incident angle as a function of β_{12} for various ω_{12} (or m_{12}). Identical system parameters are used as those given in Fig. 1.

almost linearly from positive to negative as the increasing of ω_{12} (or β_{12}) when there is no influence of other off-diagonal ones, while the effect of m_{12} is completely on the contrary. Supposing the diffusion takes place in a 2D $x_1 - x_2$ PES and x_1 is the potential valley direction, it implies that the non-orthogonality of the potential-curvature (or the friction) makes the average diffusion path of the particle to turn toward the negative x_2 axis, while the asymmetry of the inertia has a opposite affection. This reveals, in a certain reactive process, the optimal incident angle may to some extent be controlled by the varying of the non-orthogonality of the system tensors. The co-operation of the three off-diagonal system tensors may lead to a relatively ideal dynamical reactive path for the particle to surmount the barrier.

In order to get more detailed information, we made a thorough analysis about the influence of the non-orthogonality on the reactive dynamics by considering simultaneously the varying of all the three off-diagonal components. In Fig. 2, the optimal incident angle is plotted as a function of β_{12} for various ω_{12} (or m_{12}) at certain m_{12} (or ω_{12}). A common character is found as that the optimal incident angle decreases almost linearly as the increasing of β_{12} . However the decaying rate is discordance in each subgraph. An important conclusion can be made by comparing each curve in Fig. 2 as that for a reactive system with definite off-diagonal friction tensor the non-orthogonality of the potential-curvature or symmetry of the inertia could help the diffusing particle to obtain a big probability to pass the barrier. This is of directive significance in the simulation or experimental operation of many reactive processes such as the fusion of massive nuclei because accordingly one could try to select symmetric collision and non-orthogonal approximation of the potential to obtain an ultimate fusion probability.

For comparison, in Fig. 3, the optimal incident angle is plotted as a function of ω_{12} (or m_{12}) for various β_{12} . From which we can see, the optimal incident angle decreases (or increases) almost linearly with the increasing of ω_{12} (or m_{12}) at various rates. But noticing in subgraphs Fig. 3 (a) and (c) a large value of β_{12} makes it easy for the optimal incident angle to reach zero (the potential valley direction) while in subgraphs Fig. 3 (b) and (d) a small β_{12} is appreciated. This reveals, given the potential and inertia asymmetry is definite, the influence of the non-orthogonality of friction on the diffusion process is relatively complicated. This is comprehensible in the fusion process of massive nuclei. From the view point of diffusion induces fusion reaction, the friction of a reactive system relies mostly on the

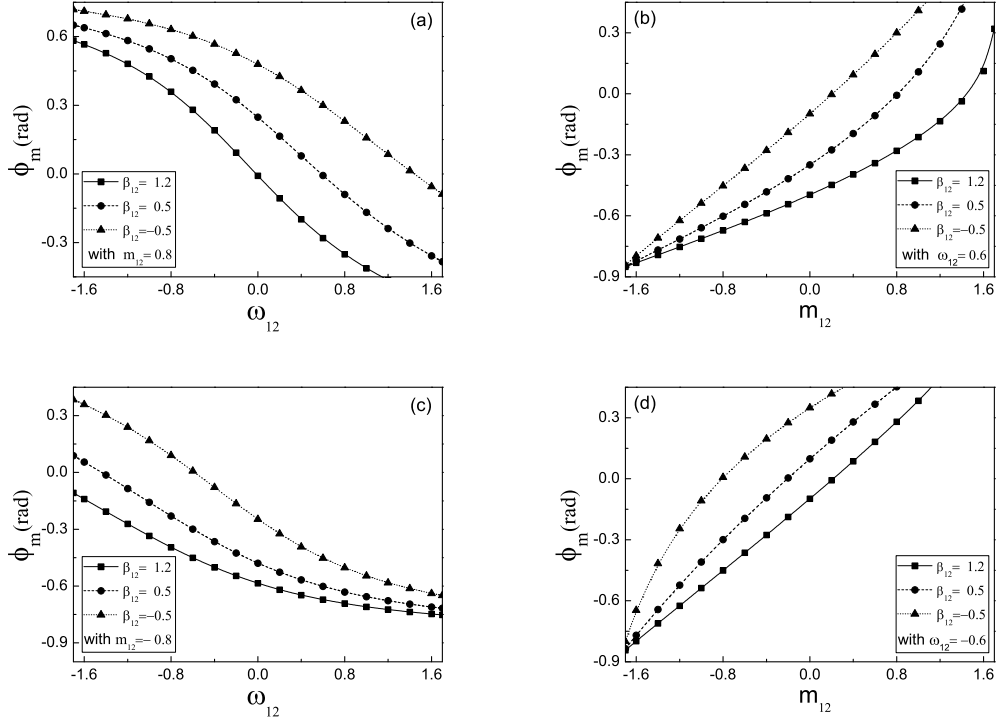


FIG. 3: Optimal incident angle as a function of ω_{12} (or m_{12}) for various β_{12} . Identical system parameters are used as those given in Fig. 1.

coupling between the system and the bath environment. In the 2D case we concerned, the strength of friction is also restricted by the coupling between two degrees of freedom. Thus results in for the diffusing particle a time-dependent or coordinate-dependent environment which makes the barrier surmounting process complicate.

III. POTENTIAL VALLEY RETURNING OF THE OPTIMAL PATH

In order to have a deep comprehension on this phenomenon, we consider a type of time-dependent system friction resulted from the non-Ohmic power spectral density $J_{ij}(\omega) = \gamma_{ij}(\omega/\omega_r)^\delta$ [9–12], where δ is the power exponent taking values between 0 and 2 in which $\delta = 1.0$ corresponds to the Ohmic damping case discussed above. γ_{ij} is the symmetrical friction constant tensor, and ω_r denotes a reference frequency induced in order to ensure the components of γ_{ij} to have the dimension of a viscosity at any δ . This kind of non-Ohmic damping can describe a large group of anomalous diffusions [13–15].

The leading part in the following discussion is still based on the optimal incident angle. In

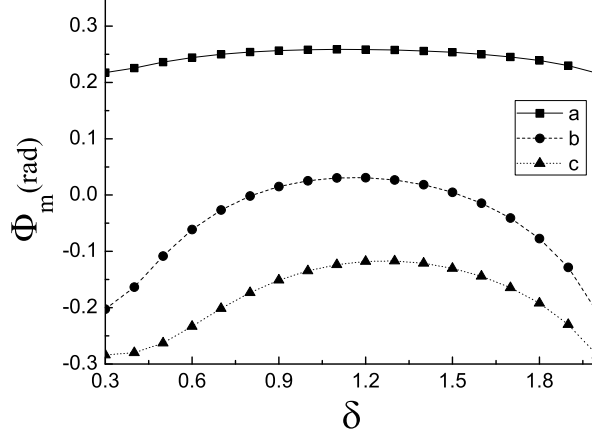


FIG. 4: Non-Ohmic optimal incident angle as a function of the power exponents δ for various effective frictions. The system parameters for each curve are (a) $\gamma_{12} = 0.8$, $\gamma_{11} = 1.8$, $\gamma_{22} = 1.2$; (b) $\gamma_{12} = 2.0$, $\gamma_{11} = 2.5$, $\gamma_{22} = 2.2$; (c) $\gamma_{12} = 4.0$, $\gamma_{11} = 4.8$, $\gamma_{22} = 4.2$, with $\omega_{12} = -0.5$ and $m_{12} = 0.6$ except those diagonal components of each tensor as those given in Fig. 1.

the non-Ohmic damping case it can be obtained by a simple generalization from Eqs.(1)-(3) with all the components of friction β_{ij} ($i, j = 1, 2$) replaced by the corresponding Laplacian transformation $\hat{\beta}_{ij}[s] = \tilde{\gamma}_{ij}s^{\delta-1}$ [6]. Where $\tilde{\gamma}_{ij} = \gamma_{ij}\omega_r^{1-\delta}\sin^{-1}(\delta\pi/2)$ is the effective friction with each component of γ_{ij} being supposed to be a constant independent of δ . Thus the optimal incident angle in the non-Ohmic case reads

$$\Phi_m = \arctan \left(\frac{m_{12}(\hat{\beta}_{22}[s]a + \omega_{22}) - m_{22}(\hat{\beta}_{12}[s]a + \omega_{12})}{m_{11}F_1(a) + m_{12}F_2(a)} \right), \quad (4)$$

implicitly containing the power exponent δ .

In Fig. 4, the non-Ohmic optimal incident angle Φ_m is plotted as a function of exponent δ at various strengths of effective frictions. In which it is revealed that the non-Ohmic optimal incident angle evolves as a non-monotonic function of the exponent δ . Given the effective friction is relatively strong (seen line (b) and (c) in Fig. 4 for example) the optimal incident angle tends to approach zero as δ is varying from non-Ohmic region to Ohmic case ($\delta = 1.0$). This is an un-trivial behavior because $\Phi_m = 0$ represents the potential valley direction. So an amazing prediction can be made as that the optimal diffusion path will in some case return to the potential valley as is always expected in the 1D model. It is also distinguished from the 2D Ohmic damping case where the optimal diffusion path is usually considered

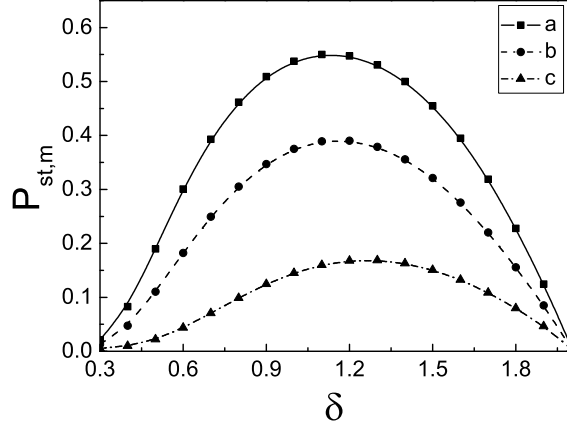


FIG. 5: The maximum stationary passing probability as a function of the power exponents δ for various effective frictions. Identical system parameters are used as those in Fig. 4.

deviating from the potential valley direction[5]. This can be understood from the view point of combined influence of the non-orthogonality of system tensors and the coupling resulted 2D non-Ohmic damping environment. It is their combination who lead the returning of 2D non-Ohmic optimal diffusion path to the potential valley.

This can also be understood by investigating the stationary barrier passing probability of the particle which is usually known as a supplemented complement error function $P_{st} = \frac{1}{2}\text{Erfc}[-\langle x_1(t) \rangle / \sqrt{2}\sigma_{x_1}(t)]$ of the reactive degree of freedom denoted as x_1 here [6]. In fig. 5 we plot the maximum value of stationary barrier passing probability $P_{st,m}$ (it can be got by tracing the particle along the optimal path) as a function of the power exponents δ for various effective frictions. From which we can see, at most cases of non-Ohmic damping ($\delta \neq 1.0$) the maximum stationary barrier passing probability is smaller than the Ohmic damping case ($\delta = 1.0$) except for a narrow range of $1.0 < \delta < 1.4$. This is because different values of power exponent δ results in different values of critical initial velocity. For example, one can find $v_0^c|_{\delta=1.8} \cong 2.6417 > v_0^c|_{\delta=0.6} \cong 2.3477 > v_0^c|_{\delta=1.0} \cong 1.8426$, while $v_0^c|_{\delta=1.1} \cong 1.8251 < v_0^c|_{\delta=1.0} \cong 1.8426$, calculated by using of the system parameters presented in Fig. 4(a) and incident angle $\Phi = 0.258\text{rad}$. Thus it results in the non-monotonic behavior of the maximum stationary barrier passing probability $P_{st,m}$ and then the potential valley returning of the optimal path.

Although it is not the primary purpose of this work, determination of the fusion probability is very important in the study of fusion dynamics. The potential valley returning behavior of the optimal path revealed in present study will provide very useful information for the experimental studying of a real reactive process. This is because one can accordingly select the most appropriated combination of the non-orthogonality of system tensors or try to make some possible adjustment on the dissipative environment to obtain a big fusion probability. For example, symmetric collision and non-orthogonal approximation of the potential in Ohmic damping environment and suitable friction strength in non-Ohmic case are appropriated as revealed in our study.

IV. SUMMARY

In conclusion of this paper, the barrier passage problem of a particle diffusing in a 2D non-orthogonal PES is studied in the framework of statistical Langevin reactive dynamics. In the whole range of friction strength from Ohmic to non-Ohmic damping, the optimal incident angle of the diffusing particle is found to be greatly influenced by the non-orthogonality of the system tensors. A type of potential valley returning behavior of the optimal path is witnessed in the 2D non-Ohmic damping environment under the combined influence of off-diagonal system tensors and the coupling between the two degrees of freedom. The result of this work provides useful information to the study of stochastic dynamical reactive processes such as the fusion of massive nuclei and those in connection with the synthesis of super-heavy elements.

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